

8. A Henry's Law Constants Database for Environmentally Significant Compounds

D.L. Poster, M.M. Schantz, H.A. Bamford, and J.E. Baker (Univ. of Maryland)

Objective: To review critically and measure Henry's Law constants for environmentally significant compounds.

Problem: Physical property data for many hazardous organic contaminants listed in the U.S. EPA's Clean Air Act Amendment of 1990 are required by a wide range of communities, including those involved with (a) implementing environmental clean-up programs, (b) modeling the fate and distribution of organic compounds in the environment, and (c) assessing human health and environmental effects associated with exposure to pollutants. However, physical property data of organic contaminants are lacking or largely inadequate for estimating their environmental behavior. Large portions of physical constant data are suspect because reported values were made at lower levels of sophistication than available today.

Approach: A physical property database for environmentally significant compounds will consist of data obtained from the literature and from measurements. The literature review will collect references that contain information on physical constants such as, surface area, heat of fusion, entropy of fusion, aqueous solubility, vapor pressure, and Henry's Law constant, and will document the measurement techniques used. One hundred twenty two references are reviewed for a wide range of compounds (Table 1). Reported values and the methods used to derive these values are extracted. Only references that contained data resulting from direct measurements are tabulated. Papers that replicate data from primary sources, are listed in the bibliography of the review. In the data compilation, each compound's Chemical Abstract Service number, molecular weight, physical constant value, method of measurement, and temperature of measurement are listed. Laboratory measurements were conducted to assess data for a range of PAHs and PCBs. Henry's Law constants were measured with equilibrium methods using assays with sufficient sensitivity for infinitesimally dilute solutions of contaminants. Simultaneous measurements of gaseous and dissolved concentrations near those found in the environment were made. Investigations of the temperature dependence of Henry's Law constants

quantified temperature effects on the air-water distribution of 13 PAHs and 24 PCBs. The temperature dependence of the Henry's law constant for each compound is modeled using the van't Hoff equation to calculate the enthalpy and entropy of volatilization. These data can be used to extrapolate the Henry's law constants within the experimental temperature range, a unique part of this work. The experimental temperature range chosen represents temperatures within environmental systems.

Table 1. Physical Property Database Compounds	
Compound Class	Number of Compounds
Polycyclic aromatic hydrocarbons (PAHs)	33
Chlorinated aliphatic compounds	19
Polychlorinated biphenyl congeners (PCBs)	152
Chlorinated benzenes	13
Polychlorinated dibenzo-pdioxins	16
Polychlorinated dibenzofurans	56

Results and Future Plans: This physical property database contains 289 organic contaminant compounds. Henry's law constants for 13 PAHs and 26 PCBs have been experimentally determined between 4°C and 31°C. These data represent the first experimentally measured temperature dependence of the Henry's law constant for 9 of the 13 PAHs and 24 of the 26 PCBs. After using relationships between temperature and the Henry's law constants for interpreting the thermodynamic relationship between the enthalpy (ΔH) and entropy (ΔS) of phase change for these compounds, this program will be concluded.

Publications:

Bamford, H.A., Poster, D.L., Baker, J.E. 1999. *Method for measuring the temperature dependence of the Henry's law constant of selected polycyclic aromatic hydrocarbons*. Polycyclic. Aromat. Compd. In Press.

Bamford, H.A., Poster, D.L., Baker, J.E. 1999. *Temperature dependence of the Henry's Law Constants of Thirteen Polycyclic Aromatic Hydrocarbons Between 4°C and 31°C*. Environ. Toxicol. Chem., 18:1905-1912

Bamford, H.A., Baker, J.E., Poster, D.L. 1998. *Review of methods and measurements of selected hydrophobic organic contaminant aqueous solubilities, vapor pressures, and air-water partition coefficients*. NIST Special Publication 928, Gaithersburg, MD.